

# D-wave overlapping band model for cuprate superconductors

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Within the BCS framework a multiband model with d-wave symmetry is considered. Generalized Fermi surface topologies via band overlapping are introduced. The band overlap scale is of the order of the Debye energy. The order parameters and the pairing have d-wave symmetry. Experimental values reported for the critical temperatures  $T_c(x)$  and the order parameters,  $\Delta_0(x)$ , in terms of doping  $x$  are used. Numerical results for the coupling and the band overlapping parameters in terms of the doping are obtained for the cuprate superconductor  $La_{2-x}Sr_xCuO_4$ .

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## I. INTRODUCTION

Measurements of angle-resolved photoemission spectroscopy (ARPES)[1] and tunneling[2], provide enough evidence for the relevant role of phonons in high- $T_c$  superconductivity (HTSC). Experimental data accumulated so far for the high- $T_c$  copper-oxide superconductors have given some useful clues to unravel the fundamental ingredients responsible for the high transition temperature  $T_c$ . However, the underlying physical process remains unknown. In this context, it seems crucial to study new ideas that use simplified schematic models to isolate the mechanism(s) that generate HTSC.

Pairing symmetry is an important element toward understanding the mechanism of high- $T_c$  superconductivity. Although early experiments were consistent with s-wave pairing symmetry, recent experiments suggest an anisotropic pairing behavior[3]. For many cuprate superconductors it is generally accepted that the pairing symmetry is d-wave for hole-doped cuprate superconductors[4] as for electron doped cuprates[5]. On the other hand, recent experiments with Raman scattering and ARPES[6, 7] have shown that the gap structure on high- $T_c$  cuprate superconductors, as a function of the angle, is similar to a d-wave gap[8, 9]. The small but non-vanishing isotope effects in high- $T_c$  cuprates have been shown compatible with d-wave superconductivity[10]. A phonon-mediated d-wave BCS like model has recently been presented to describe layered cuprated superconductors[11]. The last model account well for the magnitudes of  $T_c$  and the oxygen isotope exponent of the superconductor cuprates. Calculations with BCS theory and van Hove scenario have also been done with d-wave pairing[12]. The validity of d-wave BCS formalism in high- $T_c$  superconductor cuprates has been supported by measurements of transport properties and ARPES[13].

Numerous indications point to the multiband nature

of the superconductivity in doped cuprates. The agreement of the multiband model with experimental findings, suggests that a multiband pairing is an essential aspect of cuprate superconductivity[14].

First principle calculations show overlapping energy bands at the Fermi level[15]. The short coherence length observed in high- $T_c$  superconductors, has been related to the presence of overlapping energy bands[16, 17]. A simple model with generalized Fermi surface topologies via band overlapping has been proposed based on indirect experimental evidence. That confirms the idea that the tendency toward superconductivity can be enhanced when the Fermi level lies at or close to the energy of a singularity in the density of states (DOS)[18]. This model that can be taken as a minimal singularity in the density of states and the BCS framework, can lead to higher  $T_c$  values than those expected from the traditional phonon barrier. In our model, the energy band overlapping, modifies the DOS near the Fermi level allowing the high  $T_c$  values observed. A similar effect can be obtained with other mechanisms as a van Hove singularity in the density of states[19].

The high- $T_c$  copper-oxide superconductors have a characteristic layered structure: the  $CuO_2$  planes. The charge carriers in these materials are confined to the two dimensional (2D)  $CuO_2$  layers[20]. These layering structures of high- $T_c$  cuprates suggest that two-dimensional physics is important for these materials[11].

In this work, within the BCS framework, a phonon mediated d-wave model is proposed. The gap equation (with d-wave symmetry) and two-dimensional generalized Fermi surface topologies via band overlapping are used as a model for HTSC. A two overlapping band model is considered as a prototype of multiband superconductors. For physical consistency, an important requirement of the model is that the band overlapping parameter is not larger than the cutoff Debye energy,  $E_D$ . The model here proposed will be used to describe some properties of the cuprate superconductor  $La_{2-x}Sr_xCuO_4$  in terms of the doping and the parameters of the model.

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## II. THE MODEL

We begin with the famous gap equation

$$\Delta(k') = \sum_k V(k, k') \Delta(k) \frac{\tanh(E_k/2k_B T)}{2E_k}, \quad (1)$$

in the weak coupling limit, with  $V(k, k')$  the pairing interaction,  $k_B$  is the Boltzman constant, and  $E_k^2 = \epsilon_k^2 + \Delta_k^2$ , where  $\epsilon_k = \hbar^2 k^2/2m$  are the self-consistent single-particle energies.

For the electron-phonon interaction, we have considered, with  $V_0$  a constant,  $V(k, k') = V_0 \psi(k) \psi(k')$  when  $|\epsilon_k|$  and  $|\epsilon_{k'}| \leq E_D = k_B T_D$  and 0 elsewhere. As usual the attractive BCS interaction is nonzero only for unoccupied orbitals in the neighborhood of the Fermi level  $E_F$ . In the last equation,  $\psi(k) = \cos(2\phi_k)$  for  $d_{x^2-y^2}$  pairing. Here  $\phi_k = \tan^{-1}(k_y/k_x)$  is the angular direction of the momentum in the  $ab$  plane. The superconducting order parameter,  $\Delta(k) = \Delta(T) \psi(k)$  if  $|\epsilon_k| \leq E_D$  and 0 elsewhere.

With these considerations we propose a generalized Fermi surface. The generalized Fermi sea proposed consists of two overlapping bands. As a particular distribution with anomalous occupancy in momentum space the following form for the generalized Fermi sea has been considered

$$n_k = \Theta(\gamma k_F - k) + \Theta(\gamma k_F - k) \Theta(k - \beta k_F), \quad (2)$$

with  $k_F$  the Fermi momentum and  $0 < \beta < \gamma < 1$ . In order to keep the average number of electron states constant, the parameters are related in the 2D system by the equation

$$2\gamma^2 - \beta^2 = 1, \quad (3)$$

then only one of the relevant parameters is independent. The distribution in momentum induces one in energy,  $E_\beta < E_\gamma$  where  $E_\beta = \beta^2 E_F$  and  $E_\gamma = \gamma^2 E_F$ . We require that the band overlapping be of the order or smaller than the cutoff (Debye) energy, which means  $(1 - \gamma^2)E_F \leq E_D$ . The last expression can be written as

$$(1 - \gamma^2)E_F = \eta E_D, \quad (4)$$

where  $\eta$  is in the range  $0 < \eta < E_F/(2E_D)$ . Equations (3) and (4) together will give the minimum  $\gamma^2$  value consistent with our model.

In the last framework the summation in Eq. (1) is changed to an integration which is done over the (*symmetric*) generalized Fermi surface defined above. One gets

$$1 = \frac{\lambda}{4\pi} \int_{E_\gamma - E_D}^{E_\gamma + E_D} \int_0^{2\pi} d\phi \cos^2(2\phi) \tanh\left(\frac{\sqrt{\Xi_k}}{2k_B T}\right) \frac{d\epsilon_k}{\sqrt{\Xi_k}} + \frac{\lambda}{4\pi} \int_{E_\beta}^{E_F} \int_0^{2\pi} d\phi \cos^2(2\phi) \tanh\left(\frac{\sqrt{\Xi_k}}{2k_B T}\right) \frac{d\epsilon_k}{\sqrt{\Xi_k}}. \quad (5)$$

In this equation  $\Xi_k = (\epsilon_k - E_F)^2 + \Delta(T)^2 \cos^2(2\phi)$ , the coupling parameter is  $\lambda = V_0 D(E)$ , with  $D(E)$  the electronic density of states, which will be taken as a constant for the 2D system in the integration range.  $E_F = \frac{\hbar^2 \pi}{m} n_{2D}$ , with  $n_{2D}$  the carriers density per  $CuO_2$  layer. The two integrals correspond to the bands proposed by Eq. (2).

The integration over the surface at  $E_\gamma$  in the first band, is restricted to states in the interval  $E_\gamma - E_D \leq E_k \leq E_\gamma + E_D$ . In the second band, in order to conserve the particle number, the integration is restricted to the interval  $E_\beta \leq E_k \leq E_F$ , if  $E_\gamma + E_D > E_F$ , with  $E_\beta = (2\gamma^2 - 1)E_F$ , according to Eq. (3) in our model. While  $E_F - E_\gamma \leq E_D$ , implies that the energy difference between the anomalously occupied states must be provided by the material itself. Finally  $\Delta(T) \psi(k) = \Delta(T) \cos(2\phi)$  at the two bands.

The critical temperature is introduced via the Eq. (5) at  $T = T_c$ , where the gap becomes  $\Delta(T_c) = 0$ . At this temperature Eq. (5) is reduced to

$$1 = \frac{\lambda}{4} \int_{E_\gamma - E_D}^{E_\gamma + E_D} \tanh\left(\frac{\epsilon_k - E_F}{2k_B T_c}\right) \frac{d\epsilon_k}{\epsilon_k - E_F} + \frac{\lambda}{4} \int_{E_\beta}^{E_F} \tanh\left(\frac{\epsilon_k - E_F}{2k_B T_c}\right) \frac{d\epsilon_k}{\epsilon_k - E_F}, \quad (6)$$

which will be numerically evaluated. The last equation relates  $T_c$  to the coupling constant  $\lambda$  and to the anomalous occupancy parameter  $\gamma^2$ . This relationship determines the  $\gamma^2$  values which reproduces the critical temperature of several cuprates in the weak coupling region.

At  $T = 0K$ , Eq. (5) will also be evaluated and  $\gamma^2$  values consistent with the numerical results of Eq. (6) will be obtained:

$$1 = \frac{\lambda}{4\pi} \int_0^{2\pi} d\phi \cos^2(2\phi) \times \left[ \sinh^{-1} \frac{k_B T_D - (1 - \gamma^2)k_B T_F}{\Delta_0 |\cos(2\phi)|} + \sinh^{-1} \frac{(1 - \gamma^2)k_B T_F + k_B T_D}{\Delta_0 |\cos(2\phi)|} + \sinh^{-1} \frac{2k_B (1 - \gamma^2)T_F}{\Delta_0 |\cos(2\phi)|} \right], \quad (7)$$

where  $\Delta(0) = \Delta_0$ .

The model presented in this section can be used to describe high- $T_c$  cuprate superconductors, the band overlapping  $1 - \gamma^2$  and relevant parameters are determined. In any case a specific material must be selected to introduce the available experimental data. Ranges for the coupling parameter  $\lambda$  in the weak coupling region, and the overlapping parameter  $\gamma^2$ , consistent with the model and the experimental data, can be obtained for each material. The relationship between the characteristic parameters will be obtained for  $La$ -based compounds at several doping concentrations  $x$ , ranging from the underdoped to the overdoped regime. Different values of the

coupling constant and the overlapping parameter consistent with the model, are obtained using the experimental values of  $\Delta_0$  and  $T_c$ .

The single layer cuprate superconductor  $La_{2-x}Sr_xCuO_4$  ( $La-214$ ) has one of the simplest crystal structures among the high- $T_c$  superconductors. This fact makes this cuprate very attractive for both theoretical and experimental studies. High quality single crystals of this material are available with several doping concentrations which are required for experimental studies. Even the determination of charge carrier concentration in the cuprate superconductors is quite difficult, the  $La-214$  is a system where the carrier concentration is nearly unambiguously determined. For this material, the hole concentration for  $CuO_2$  plane,  $n_{2D}$ , is equal to the  $x$  value, *i.e.* to the  $Sr$  concentration, as long as the oxygen is stoichiometric[21, 22]. Additionally, there are reliable data for the  $T_c$  and the superconducting gap  $\Delta_0$  for several samples in the superconducting region.

### III. RESULTS AND DISCUSSION

In order to get numerical results, with our overlapping band model with d-wave symmetry, the cuprate  $La_{2-x}Sr_xCuO_4$  was selected. The values for  $\Delta_0$  are taken in the interval  $2 \leq \Delta_0 \leq 12$  meV which includes experimental results[22]. The behavior of  $\lambda$  as function of  $x$  and  $\gamma^2$  at  $T = T_c$  is obtained from Eq. (6); and  $\lambda$  as function of  $\Delta_0$ ,  $x$  and  $\gamma^2$  at  $T = 0K$  is given by Eq. (7). To have coupled solutions of these equations the same  $\lambda$  value for  $T = T_c$  and  $T = 0K$  is proposed. These solutions correspond to different overlap values  $1 - \gamma^2$ , at each equation. With this model and s-wave symmetry, the band overlapping  $1 - \gamma^2$  was higher at  $T = 0K$  than at  $T = T_c$ [23]. We consider the same behavior with d-wave symmetry. The maximum  $T_c$  for cuprate superconductors is obtained at optimal doping. With the model  $\lambda(x)$  values are obtained, including at optimal doping  $\lambda(x_{op})$ [24].

In Fig. 1. values of the coupling parameter  $\lambda$  in terms of the overlapping parameter  $\gamma^2$  are shown in the weak coupling region. The experimental results of  $T_c$  and  $\Delta_0$  from Refs. [20] and [22] were introduced. The curves at  $T = 0K$  (broken curve) and at  $T = T_c = 40K$  (continuous curve) for  $La_{2-x}Sr_xCuO_4$ , with optimal doping  $x_{op} = 0.16$  are shown. The minimum  $\gamma^2$  value of 0.55 was taken to be consistent with the model. In the whole range reported for the band overlapping, the coupling parameter required at each  $\gamma^2$  is larger for  $T = 0K$  than for  $T = T_c$ . In order to use the same  $\lambda$  for  $T = T_c$  and  $T = 0K$ , the  $\lambda$  values must be restricted *i.e.*, the  $\lambda$  value at each  $\gamma^2$  must be larger than  $\lambda_{min} = 0.57$  at  $T = 0K$ .

In the region  $\gamma^2 \geq 0.7$  with a constant  $\lambda$  value, a larger band overlapping  $1 - \gamma^2$  is obtained for  $T = 0K$  than for

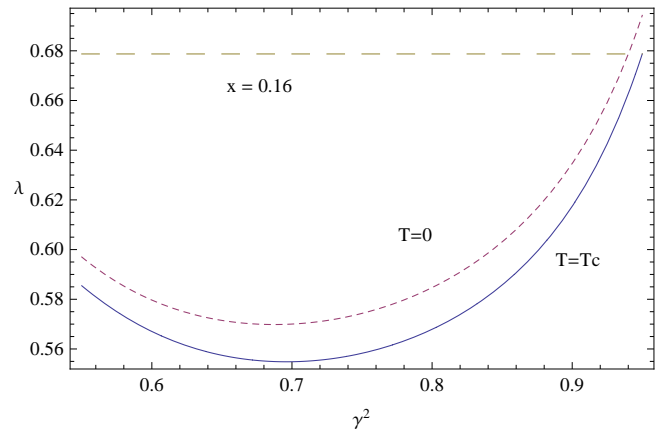


FIG. 1: The coupling parameter  $\lambda$  in terms of the overlapping parameter  $\gamma^2$ , with optimal doping  $x = 0.16$ . The  $T = 0K$  (broken curve) and  $T = T_c = 40K$  (continuous curve) for  $La_{2-x}Sr_xCuO_4$ , are shown. The horizontal line at  $\lambda = 0.68$  shows the maximum  $\lambda$  selected for  $T = T_c$  with  $\gamma^2 = 0.95$ .

$T = T_c$  in agreement with our assumption. For instance, the maximum  $\lambda$  for  $T = T_c$  with  $\gamma^2 = 0.95$ , is shown by the horizontal line at  $\lambda = 0.68$ , and the intersection of this line and the  $T = 0K$  curve is at  $\gamma^2 = 0.94$ . The same restrictions over  $\lambda$  are considered at any other doping in the superconducting phase. However, for any  $x \neq x_{op}$ , the  $\lambda$  value must be smaller than  $\lambda = 0.68$ .

In Fig. 2 the results for optimal doping  $x_{op}$ , are compared with the underdoped  $x = 0.13$  and the overdoped  $x = 0.2$  cases. The experimental values of  $\Delta_0$  and  $T_c$  for each doping, were introduced. The continuous curves correspond to  $x_{op}$ , the small dashed curves show the underdoped behavior and the large dashed ones the overdoped results. In the optimally doped and underdoped cases, the  $T = 0K$  curves are above the corresponding  $T = T_c$  ones. In the overdoped case, the behavior is different *i.e.*, the  $T_c$  curve is above the  $T = 0K$  one.

In the three cases, the values of the coupling parameter are in the weak coupling region for the  $\gamma^2$  values which satisfy the conditions of our model. All the  $\gamma^2$  values which satisfy the  $\lambda$  restrictions are allowed. However, as an example, we have selected extreme  $\lambda$  values in the three cases. The three horizontal lines show these  $\lambda$  values.

As in Fig. 1 the maximum  $\lambda$  value selected at optimal doping is  $\lambda = 0.68$ . In the underdoped case  $\lambda = 0.65$  is selected. This value corresponds to the overlapping parameter  $\gamma^2 = 0.621$ , the minimum of the  $T = 0K$  curve, and  $\gamma^2 = 0.941$  at the  $T = T_c$  curve. In the overdoped case, the selected  $\lambda$  value is 0.51, *i.e.* the minimum of the curve  $T = T_c$ . With this  $\lambda$ , the overlapping parameters are  $\gamma^2 = 0.599$  for  $T = 0K$  and  $\gamma^2 = 0.76$  for  $T = T_c$ .

With numerical solutions of Eq. (7) we may obtain the gap  $\Delta_0$  in terms of the parameters of our model. The

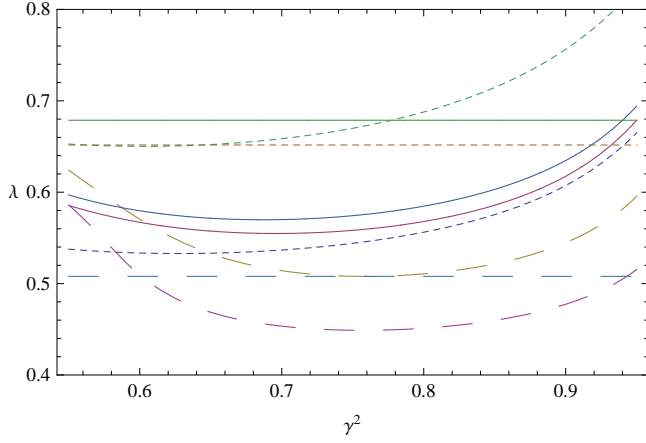


FIG. 2: The results for optimal doping (continuous curves) are compared with the underdoped (small dashed curves)  $x = 0.13$  and the overdoped  $x = 0.2$  (large dashed curves) cases. The three horizontal lines show the selected extreme  $\lambda$  values:  $\lambda = 0.68$  at optimal doping,  $\lambda = 0.65$  in the underdoped case, and  $\lambda = 0.51$  in the overdoped case.

underdoped material is considered in Fig. 3 because the advantage of our model is easily shown. The gap  $\Delta_0$  is shown in terms of the coupling parameter  $\lambda$ . The gap  $\Delta_0$  always increases with the coupling parameter  $\lambda$ . The curves are drawn for  $\gamma^2 = 0.621, 0.5$  and  $0.8$  from up to down respectively. For this sample, with  $\gamma^2 = 0.621$ , we obtain the minimum  $\lambda$  value for any  $\Delta_0$  and for any  $\lambda$  the maximum  $\Delta_0$  value.

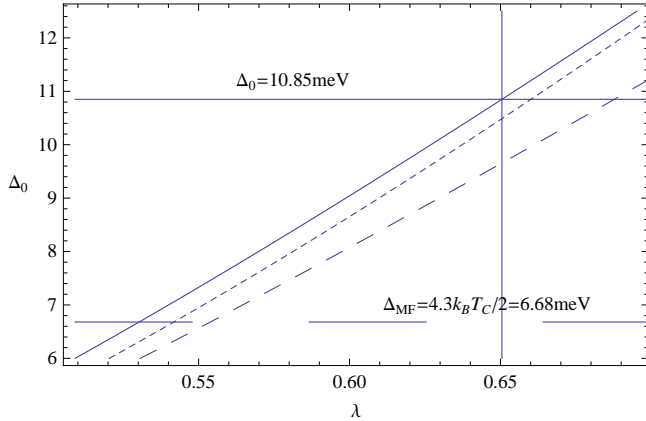


FIG. 3: The gap  $\Delta_0$  obtained in terms of the coupling parameter  $\lambda$  for the underdoped sample. The curves are drawn for  $\gamma^2 = 0.621, 0.5$  and  $0.8$  from up to down respectively. The continuous horizontal line shows the experimental  $\Delta_0 = 10.85\text{meV}$  value. The large dashed horizontal line shows the d-wave mean-field approximation  $\Delta_{MF} = 6.68\text{meV}$  result.

The continuous horizontal line shows the experimental  $\Delta_0 = 10.85\text{meV}$  value. The large dashed horizontal line shows the d-wave mean-field approximation

$\Delta_{MF} = 6.68\text{meV}$  result[25], where the same d-wave symmetry was considered. However, introduction of the band overlapping allows to reproduce the experimental result with all the  $\gamma^2$  values in the range considered. The band overlapping model also allows higher  $\Delta_0$  values for the underdoped system and lower  $\Delta_0$  for the overdoped one, than the  $\Delta_{MF} = 2.145k_B T_c$ .

In Fig. 4 the behavior between  $\Delta_0$  and  $\lambda$  for optimal doping is compared with the underdoped and the overdoped cases. The  $\gamma^2$  values introduced are those selected in Fig. 2 for  $T = 0\text{K}$ . The horizontal lines are the  $\lambda$  values also selected in Fig. 2. All the continuous curves correspond to optimal doping. The large and small dashed curves correspond to the overdoped and the underdoped systems respectively. The curves show the interesting relationship between these parameters. As for optimal doping, the coupling parameter increases with  $\Delta_0$  for any doping. The vertical lines are the experimental  $\Delta_0$  values. It is possible to reproduce the experimental  $\Delta_0$  in the range  $0.13 \leq x \leq 0.2$ . The band overlapping introduced in this model allows the reproduction of the behavior of  $\Delta_0$  with doping.

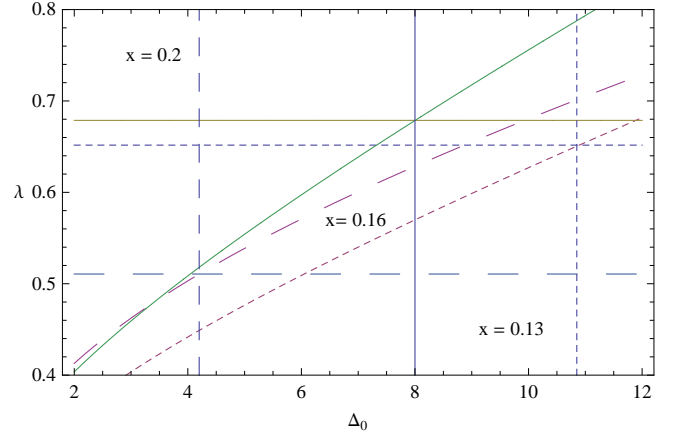


FIG. 4:  $\Delta_0$  as function of  $\lambda$  for optimal doping, underdoped, and the overdoped cases. The horizontal lines are the  $\lambda$  values selected in Fig. 2. The vertical lines show the experimental  $\Delta_0$  values. The continuous lines correspond to  $x = 0.16$ , the small dashed ones to  $x = 0.13$ , and the large dashed ones to  $x = 0.2$ .

In conclusion, we presented an overlapping band model with d-wave symmetry, to describe high- $T_c$  cuprate superconductors, within the BCS framework. We have used a model with anomalous Fermi Occupancy and d-wave pairing in the 2D fermion gas. The anomaly is introduced via a generalized Fermi surface with two bands as a prototype of bands overlapping. We report the behavior of the coupling parameter  $\lambda$  as function of the gap  $\Delta_0$  and the overlapping parameter  $\gamma^2$ , for different doping samples. The  $\lambda$  values consistent with the model are in the weak coupling region. The behavior of  $\Delta_0$  as function

of  $\lambda$  shows that for several band overlapping parameters it is possible to reproduce the experimental  $\Delta_0$  values near the optimal doping, for the cuprate  $La_{2-x}Sr_xCuO_4$ . The band overlapping allows the improvement of the results obtained with a d-wave mean-field approximation, in a scheme in which the electron-phonon interaction is the relevant high- $T_c$  mechanism. The energy scale of the

anomaly  $(1 - \gamma^2)E_F$  is of the order of the Debye energy. The Debye energy is then the overall scale that determines the highest  $T_c$  and gives credibility to the model because it requires an energy scale accessible to the lattice. The enhancing of the DOS with this model simulates quite well intermediate and strong coupling corrections to the BCS framework.

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